NETL-RUA
Regional University Alliance

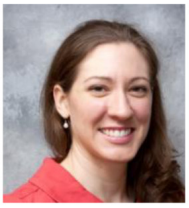
E NEWS

Shared Intellect • Shared Laboratories • Shared Resources

September 2012
VOLUME 2, ISSUE 8

NETL-RUA Members Selected as Ambassadors in Pilot Science Program


George Guthrie


Alexandra Hakala


Brian Gleeson


Gregory Reed


Edward Rubin


Neil Donahue


Jay Apt


Paul Ohodnicki


Bryan Morreale


Christina Gabriel

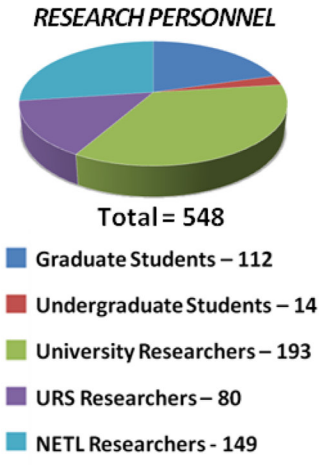
On Wednesday, May 30, the National Academy of Sciences (NAS) and the National Academy of Engineering (NAE) named Pittsburgh as the site for their Science & Engineering Ambassador Program. The focus of this pilot program is energy, making Pittsburgh an obvious choice as it has become a nexus for the coal, natural gas,

>> *See* **AMBASSADORS**, *Page 2*

NETL-RUA METRICS SNAPSHOT

PRODUCTS		
	FY2011	FY2012
Publications	194	70
Patents	11	2
Licenses	9	4
Students Graduated	20 PhD	23 PhD
	8 MS	18 MS

Product data is updated quarterly.



E News is your monthly source for the latest information about NETL-RUA's research, activities, and other important news. If you have information that you would like to feature in future newsletters, send that information to

paul.deffenbaugh@contr.netl.doe.gov
or
jane.engel@contr.netl.doe.gov

What's in This Issue

The FY11 NETL-RUA Annual Review is complete and has been posted to the

Member's Only SharePoint Site (MOSS)

Contact:

Julianne Klara
julianne.klara@netl.doe.gov
412-386-6089

>> **AMBASSADORS**, *Continued from Page 1*

nuclear, solar, and wind power industries and research. Additionally, Pittsburgh is the home to an impressive number of eminent energy-related scientists and engineers in some of the nation's top universities.

The goal of the program is to raise awareness about energy issues and help community members such as teachers, business leaders, and local media groups become comfortable with discussing energy issues with the community. The ambassadors are established, well-respected experts who come from academia, industry, or government, and several Pittsburgh scientists and engineers have been selected as ambassadors to promote this goal. In fact, a majority of the ambassadors are NETL-RUA members, including Jay Apt, Neil Donahue, and Edward S. Rubin from Carnegie Mellon University; Brian Gleeson and Gregory Reed from the University of Pittsburgh; Christina Gabriel, President of the University Energy Partnership (UEP) and a member of the NETL-RUA Executive Committee (EC); and George Guthrie, Bryan Morreale, Alexandra Hakala, and Paul Ohodnicki of NETL.

The long-term goal of the two academies is to develop a replicable model of the program that can be implemented in cities nationwide, building stronger relationships between scientists/engineers and their communities while improving citizens' engagement with current issues in science, technology, and medicine.

Join Us Online

Your favorite issues of the NETL-RUA E NEWS are now available on the Members Only SharePoint Site

External Awards Bring International Awareness

NETL places heavy emphasis on the pursuit of scientific and engineering recognition awards. These efforts result in more than a dozen awards per year for federal employees and their collaborative partners. Award opportunities represent an avenue for researchers and research teams to be publicly recognized for outstanding work and accomplishments both here in the U.S. and around the world.

Most recently, prestigious awards such as the R&D 100, DOE Secretarial Awards, and Excellence in Government Awards have been granted to researchers associated with NETL. Thus far for FY2012, twelve awards have been received for individual and team nominations.

In an effort to consider alternative ways to recognize the unique collaboration of the NETL-RUA, researchers are encouraged to pursue opportunities through professional organizations, associations, and scientific societies. Organizations such as the American Chemical Society (ACS), Materials Research Society (MRS), American Institute for Chemical Engineers (AIChE), American Physical Society (APS), American Society for Materials International (ASM), and American Society of Mechanical Engineers (ASME) sponsor awards as well as other recognitions such as "fellow" of a scientific society. The NAS and NAE honor significant achievements by selecting members of these very prestigious and influential organizations.

Members of the NETL-RUA who are qualified for nomination or interested in nominating another person or team for these types of awards should contact Nancy Andres at 412-386-5705.

2012 Award Recipients to Date:

Dave Berry

James Bennett

Ben Chorpening

McMahan Gray

Ale Hakala

Dave Huckaby

John Kitchin

Ken Lyons

Jinichiro Nakano

Meghan Napoli

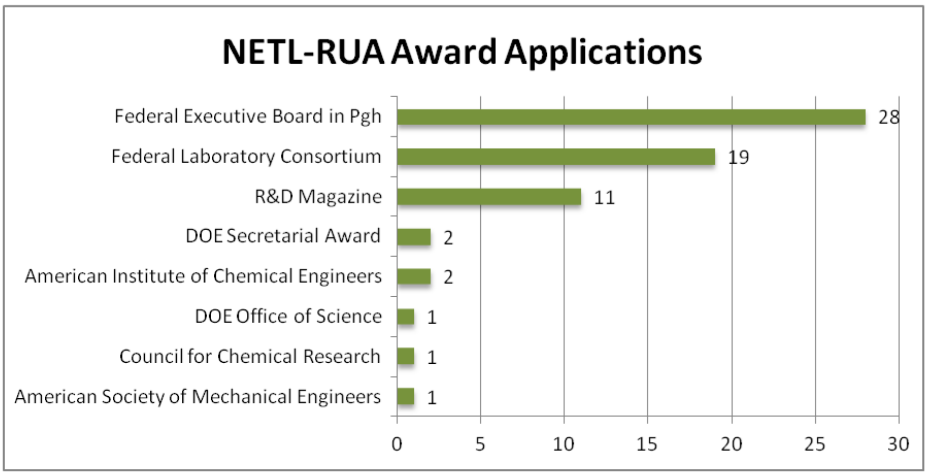
Paul Ohodnicki

Kyei-Sing Kwong

Bob Warzinski

Gas Hydrate Team

Raman Team



NETL-RUA Researcher Wins HENAAC Award

NETL-RUA researcher Dr. Alexandra "Ale" Hakala has been honored with the Great Minds in STEM™ Hispanic Engineer National Achievement Awards Corporation (HENAAC) award for Outstanding Technical Achievement.

Dr. Hakala's innovative and inspirational qualities, as well as her drive, are just a few of the reasons she was chosen for this award. According to NETL Director Anthony Cugini, in just three years as a research scientist at NETL, "Dr. Hakala has emerged as a talented scientist, gifted leader, and an articulate ambassador for the Laboratory's research, its programs, and the importance of our work to the energy sector of the United States."

Dr. Hakala leads and participates on a number of research teams that span the NETL-RUA, focused on geochemistry-related studies for shale gas and geothermal energy resources, and geologic CO_2 storage. She is also the Technical Coordinator for shale gas research, in which role she works with multiple principal investigators to coordinate field, laboratory, and modeling investigations focused on safe and environmentally sustainable development of shale gas resources. She serves as the technical lead for the NETL-RUA Shale Gas Strategic Growth Initiative (SGA).

Ale grew up in eight different locations across the U.S., but now calls Pittsburgh home. She earned a B.A. in geosciences with a certificate in environmental studies from Princeton University (Princeton, New Jersey) and a Ph.D. from the School of Earth Sciences at The Ohio State University (Columbus, Ohio).

Dr. Hakala will receive her award at the 24th Annual HENAAC Conference, "STEM, Excellence, and the Pursuit of Innovation," on October 12, 2012. Great Minds in STEM considers nominees for their awards to be "top role models" in science, technology, engineering, and math (STEM) fields and uses the HENAAC awards to "promote and highlight Hispanic engineers and scientists." These awards spotlight rising stars in STEM to encourage the next generation to pursue careers in these fields and motivate current STEM innovators to continue to connect with their Hispanic heritage.

Upcoming Events

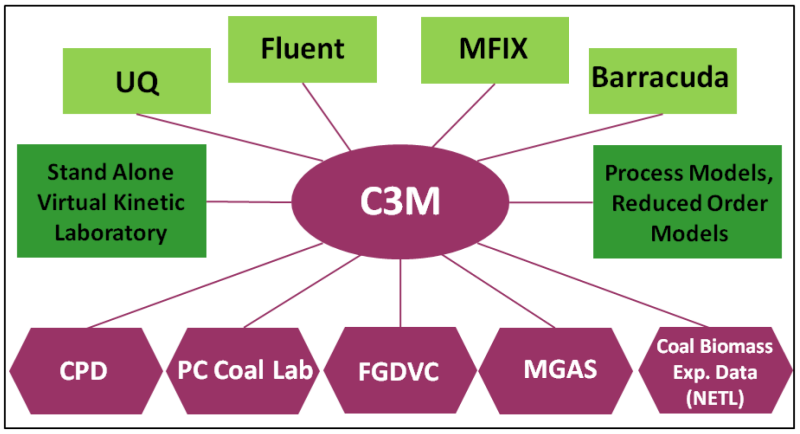
- **Materials Science & Technology 2012 Conference & Exhibition**,
  October 7–11, 2012 | David L. Lawrence Convention Center | Pittsburgh, PA
- **2012 Pittsburgh Coal Conference**,
  October 15–18, 2012 | David L. Lawrence Convention Center | Pittsburgh, PA
- **2012 AIChE Annual Meeting, Cleaner Energy, Stronger Economy, Better Living**,
  October 28–November 2, 2012 | David L. Lawrence Convention Center | Pittsburgh, PA
- **NETL-RUA Fall Meeting: Energy & Innovation Conference**,
  November 28–29, 2012 | Southpointe Hilton Garden Inn | Canonsburg, PA

Look for more information on these events in upcoming issues of the newsletter

Technology Spotlight

Carbonaceous Chemistry for Computational Modeling

As part of NETL-RUA's Gasification Research Team, the research being conducted by Professor Richard Turton and his team at West Virginia University (WVU) is to support the development of the NETL software platform entitled Carbonaceous Chemistry for Computational Modeling (C3M) that provides the kinetic database for the processes and reaction mechanisms typically found in coal gasification, gas clean-up, and carbon capture processes. Currently the C3M graphical user interface (GUI) has been designed to enable the user to test and update the coal devolatilization, tar cracking, secondary pyrolysis, char and soot oxidation and gasification kinetics in METC Gasifier Advanced Simulation (MGAS) with the kinetics derived from PC Coal Lab (PCCL), Chemical Percolation model for Devolatilization (CPD), Functional-Group, Depolymerization, Vaporization, Cross-linking (FG-DVC) and experimental co-pyrolysis data. In addition, computational fluid dynamics models (MFIX, ANSYS FLUENT and BARRACUDA) can be executed with the new kinetics information obtained from C3M. The figure to the right illustrates schematically how C3M currently works to provide a user-friendly GUI linking coal or other fuel chemistry and/or kinetics codes to higher level computational fluid dynamics simulations. Also shown in the figure is an uncertainty quantification (UQ) tool that is a statistical technique to develop a numerical or mathematical model to predict the uncertainty in the output based on the variations in input parameters. UQ is a unique feature that can be coupled with C3M. By utilizing a UQ toolbox (e.g., using PSUADE, DAKOTA, and SAS-JMP), the user can observe and predict the uncertainties/variations in product yields and reaction rates with the prescribed variability in operating conditions and fuel properties. This is achieved by conducting matrices of systematically designed experimental runs with the kinetic packages available in C3M and analyzing the output with the UQ toolbox. This is a very cheap and cost effective method of capturing uncertainty in the kinetic models for various fuels.



Business Development Update

The Critical Materials Hub proposal led by Virginia Tech (VT) was completed and submitted on time on August 30. This was a significant undertaking and the first of a kind for the NETL-RUA where we (1) targeted an area for strategic growth, (2) jointly supported the development of our capabilities, and (3) pooled our collective resources to pursue the capture of a program against national competition. First of a kind efforts are always challenging and we will have many lessons learned to share from the journey. Many thanks to Dr. Roe-Hoan Yoon and the VT Team for their leadership in pulling together and delivering this proposal.

Executive Committee Update

NETL-RUA Committees to be Replaced with Ad-Hoc Teams

On August 29, the NETL-RUA EC held a day-long strategic planning session to define a long-term vision for the Alliance and develop near-term goals and actions for growing the visibility, impact, and size of the NETL-RUA R&D portfolio. To support the strategic plan, the EC determined that teams provided with committed resources and chartered to accomplish the plan's specific tasks would be most effective in achieving the desired outcomes. Therefore, the existing NETL-RUA standing committees were formally dissolved in favor of ad-hoc teams that will be established by the EC as needed. Once completed, the strategic plan will be shared with NETL-RUA members.